

# A new effective interaction for the trapped Fermi gas

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We apply the configuration-interaction method to calculate the spectra of two-component Fermi systems in a harmonic trap, studying the convergence of the method at the unitary interaction limit. We find that for a fixed regularization of the two-body interaction the convergence is exponential or better in the truncation parameter of the many-body space. However, the conventional regularization is found to have poor convergence in the regularization parameter, with an error that scales as a low negative power of this parameter. We propose a new regularization of the two-body interaction that produces exponential convergence for systems of three and four particles. From the systematics, we estimate the ground-state energy of the four-particle system to be  $(5.05 \pm 0.024)\hbar\omega$ .

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The study of cold trapped atomic condensates has become a rich field experimentally. By providing a strongly interacting system that is well defined, it also offers physicists an unprecedented opportunity to assess theoretical techniques that cross the boundaries of disciplines. In the so-called unitary limit, the only dimensional scale of the problem is fixed by the harmonic trap frequency. Systematic studies have begun on small systems using fixed-node Monte Carlo [1, 2] and density functional methods [3]. Remarkably, the exact wave functions and energies of the  $A = 3$  system are known, calculated by solving a single transcendental equation [4]. Our work here is in the context of the configuration-interaction (CI) method, widely used in atomic, molecular, and nuclear spectroscopy. We study the convergence of the CI method with respect to a regularization parameter of the two-body interaction and find that a simple regularization scheme that renormalizes the interaction produces slow convergence of the three- and four-particle spectra. We introduce a new effective interaction that gives exponential convergence, at least in small systems.

*Hamiltonian.* The cold trapped atom system is modeled by the Hamiltonian

$$H = - \sum_{i=1}^A \frac{\hbar^2}{2m} \nabla_i^2 + \sum_{i=1}^A \frac{1}{2} m \omega^2 r_i^2 + \sum_{i < j} V_0 \delta(\mathbf{r}_i - \mathbf{r}_j), \quad (1)$$

where  $A$  is the number of atoms,  $\omega$  is the trap frequency, and  $V_0$  is the interaction strength. We have two-component fermionic systems in mind, which controls the symmetry of the allowed states. The interaction is represented as a  $\delta$  function (contact interaction) but as we shall see below it requires a regularization. Here we focus on an attractive contact interaction in the unitary limit of infinite scattering length.

*The two-particle problem.* The two particle system ( $A = 2$ ) is separable in center of mass and relative coordinates  $\mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1$ . The center of mass Hamiltonian describes an

harmonic oscillator with frequency  $\omega$  and mass  $2m$ , while the relative-coordinate Hamiltonian is  $H_{\text{rel}} = -\frac{\hbar^2}{2\mu} \nabla_{\mathbf{r}}^2 + \frac{1}{2} \mu \omega^2 r^2 + V_0 \delta(\mathbf{r})$  with reduced mass  $\mu = m/2$ . The two-particle energies are given by

$$E = (2\mathcal{N} + \mathcal{L} + 3/2)\hbar\omega + \varepsilon_{nl}, \quad (2)$$

where  $\mathcal{N}, \mathcal{L}$  and  $n, l$  are the radial quantum number and angular momentum of the center of mass and relative motion, respectively. The energies  $\varepsilon_{nl}$  are the eigenvalues of  $H_{\text{rel}}$ , and may be derived from the boundary condition at the origin imposed by the unitary interaction [5]. The contact interaction affects only the  $l = 0$  partial waves, and shifts each  $s$ -wave oscillator energy down by one unit of  $\hbar\omega$  [6]. Thus we have

$$\varepsilon_{nl} = (2n + l + 3/2 - \delta_{l,0})\hbar\omega; \quad n = 0, 1, 2, \dots \quad (3)$$

*The renormalized contact interaction.* In the CI method, the contact interaction in Eq. (1) must be treated explicitly. However, a  $\delta$ -function interaction cannot be used in three dimensions without a regularization. We shall do this by truncating the space of relative-coordinate wave functions to a  $q$  subspace defined by the lowest  $q + 1$  oscillator  $l = 0$  wave functions (see also Ref. [7]). Within the truncated space the relative-coordinate Hamiltonian can be written as

$$(H_{\text{rel}})_{n,n'}^{(q)} = (2n + 3/2)\hbar\omega \delta_{n,n'} + V_{n,n'}^{(q)}, \quad (0 \leq n, n' \leq q) \quad (4)$$

where

$$V_{n,n'}^{(q)} = \hbar\omega \chi_q \psi_n(0) \psi_{n'}(0), \quad (5)$$

and  $\psi_n(0) = \pi^{-3/4} \sqrt{(2n+1)!/(2^n n!)}$  is the  $(n, l = 0)$  oscillator wave function at  $r = 0$  for an oscillator of radius 1. The parameter  $\chi_q$  is a dimensionless normalization constant related to  $V_0$  by  $\chi_q = (\hbar^2/\mu)^{-3/2} (\hbar\omega)^{1/2} V_0$ .

We determine the normalization constant  $\chi_q$  by requiring the ground-state energy of the truncated Hamiltonian

to equal the exact value for the unitary contact interaction,  $\varepsilon_{00} = \hbar\omega/2$ . The separable form of (5) permits an algebraic diagonalization of the Hamiltonian. Each eigenvalue  $\varepsilon$  of (4) satisfies the dispersion formula

$$\chi_q^{-1} = -\sum_{n=0}^q \frac{\psi_n^2(0)}{(2n+3/2) - \varepsilon/\hbar\omega}. \quad (6)$$

Requiring  $\varepsilon = \varepsilon_{00} = \hbar\omega/2$  in (6), we obtain a closed expression for the normalization constant

$$\chi_q = -\pi^{3/2} \left( \sum_{n=0}^q \frac{(2n-1)!!}{2^n n!} \right)^{-1}. \quad (7)$$

We note that the sum in (7) diverges as  $q^{1/2}$  for large  $q$  [8]. Thus, the strength of the  $\delta$ -function goes to zero as  $q \rightarrow \infty$ , showing the need for a renormalization procedure. A similar relation between the strength of the interaction and the cutoff can be derived for a plane-wave basis. In that case the relation is  $V_0 = -\pi^2 \hbar^2 / \mu \Lambda$  where  $\Lambda$  is a momentum cutoff [9]. This value of  $V_0$  agrees with the asymptotic expression of Eq. (7) [8] once we equate the corresponding cutoff energies as  $\hbar^2 \Lambda^2 / 2\mu = (2q+3/2)\hbar\omega$ .

The excited states of the  $q$ -truncated Hamiltonian (4) have energies  $\varepsilon_{n0}^{(q)}$  that differ from the exact unitary spectrum (3). Using the dispersion relation (6), we find that the error in the energy  $\delta\varepsilon_{n0}^{(q)} = \varepsilon_{n0}^{(q)} - \varepsilon_{n0}$  goes to zero at large  $q$ , but only at a rather slow rate,  $\delta\varepsilon_{n0}^{(q)} \sim q^{-1/2}$ . We present evidence below that this slow convergence is also present in the  $q$ -renormalized energies for the  $A=3$  and  $A=4$  systems. This makes it problematic to extrapolate the  $q$  series to estimate the true  $q \rightarrow \infty$  energies.

*A new effective interaction.* We have considerably more freedom to construct the  $q$ -space interaction than we have exploited so far. The only requirement on the  $q$ -space Hamiltonian is that it converge to the unitary limit for large  $q$ . For example, in effective field theory one may introduce derivatives of the contact interaction to fit certain properties of the two-particle Hamiltonian. Here we propose the following prescription to improve the  $q$ -space interaction: simply require that the relative-coordinate Hamiltonian reproduce all  $q+1$   $s$ -wave eigenvalues of Eq. (3). We can do this and still keep the separable form for the interaction,

$$V_{n,n'}^{\text{eff}(q)} = -\hbar\omega f_n f_{n'}. \quad (8)$$

A motivation for preserving the separable form is given in the discussion below. There are  $q+1$  independent variables  $f_n$  in the interaction (8) and the same number of eigenvalue equations having the form of Eq. (6) with  $f_n$  replacing  $\sqrt{|\chi_q|}\psi_n(0)$ . Using the conditions that all  $q+1$  lowest  $l=0$  unitary eigenvalues (3) ( $n=0, \dots, q$ ) are reproduced, we find the following  $q+1$  equations for

$f_n$

$$\sum_{n=0}^q \frac{f_n^2}{2(n-r)+1} = 1 \quad (r=0, \dots, q). \quad (9)$$

Eqs. (9) determine a unique solution for  $f_n^2$  ( $n=0, \dots, q$ ) [10]. We choose the sign of the real numbers  $f_n$  to coincide with the sign of  $\psi_n(0)$ . Using the convention that the harmonic oscillator wave functions be positive at the origin, the unique solution for  $f_n$  is

$$f_n = \sqrt{\frac{(2n+1)!!}{(2n)!!} \frac{[2(q-n)-1]!!}{[2(q-n)]!!}}. \quad (10)$$

The interaction defined by (8) and (10) is different from the renormalized contact interaction for any  $q$ . However, its eigenfunction components (in the 3-D oscillator basis) converge to the corresponding unitary eigenfunction components in the limit of large  $q$  with an error of  $\sim q^{-1}$ . In comparison, the eigenvector components of the renormalized contact interaction converge to the same unitary eigenvector components but at a slower rate of  $\sim q^{-1/2}$ . *CI method and truncation of many-particle space.* In the CI approach, one uses a single-particle basis in the laboratory frame and constructs a many-particle basis of Slater determinants for  $A$  fermions. In our problem, a natural choice for the single-particle basis are the eigenstates of the three-dimensional harmonic oscillator. These states are labeled by orbital quantum numbers  $a = (n_a, l_a)$ , the orbital magnetic quantum number  $m_a$ , and an additional two-valued quantum number (e.g. spin) to distinguish the two species of fermions.

A way to truncate the many-particle space must be specified, because there is no natural truncation associated with the interaction except in the trivial cases  $q=0$  or  $A=2$ . There are a number of truncation schemes in the literature; here we will define a truncated single-particle orbital basis and construct the  $A$ -particle wave function allowing all possible anti-symmetrized product states. In particular, we shall use all single-particle states in the oscillator shells  $N=0, \dots, N_{\text{max}}$  with  $N=2n_a+l_a$  to construct the many-particle states. There will be two limiting processes necessary to calculate the many-particle energies. The first is  $N_{\text{max}} \rightarrow \infty$ , which we will investigate for fixed  $q$ . Then, with converged  $q$ -regulated energies we estimate the  $q \rightarrow \infty$  limit.

Two technical aspects of our calculations should be mentioned. The two-particle matrix elements of the interaction in the oscillator basis are conveniently calculated using the Talmi-Moshinsky brackets to transform to relative and center of mass coordinates [11]. The many-particle Hamiltonian is constructed and diagonalized using the nuclear shell model code `oxbash` [12]. Unlike the nuclear shell model, our orbitals are characterized by integer angular momentum values. The two fermion species are distinguished in the same way as neutrons and protons are distinguished in the nuclear application.

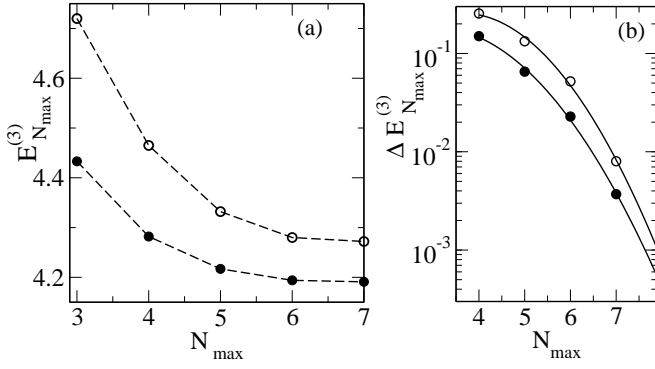


FIG. 1: Convergence in  $N_{\max}$  for the  $A = 3$  ground-state energy. (a)  $E_{N_{\max}}^{(q)}$  versus  $N_{\max}$  for  $q = 3$ . Open circles correspond to the renormalized contact interaction and solid circles to the interaction defined by (8) and (10). (b)  $\Delta E_{N_{\max}}^{(3)}$  versus  $N_{\max}$  in a logarithmic scale. All energies are in units of  $\hbar\omega$ .

*A=3 system.* We now show the results for  $A = 3$ . The ground state of the  $A = 3$  system is a negative-parity state with total angular momentum  $L = 1$  and energy  $4.2727243 \dots \hbar\omega$  [4, 13]. In our CI convergence studies we computed the ground-state energies  $E_{N_{\max}}^{(q)}$  for  $q = 1, 2, 3, 4$  and  $N_{\max} = q, \dots, 7$ .

For a fixed  $q$ , we find that  $E_{N_{\max}}^{(q)}$  converge exponentially or better in  $N_{\max}$  for both interactions. This is demonstrated in Fig. 1. Panel (a) shows  $E_{N_{\max}}^{(q)}$  versus  $N_{\max}$  for  $q = 3$ . Both the renormalized contact interaction (open circles) and the new interaction (solid circles) are monotonically decreasing, as they must when the space gets larger. The important point, seen in Fig. 1(b), is that the energy differences  $\Delta E_{N_{\max}}^{(q)} \equiv E_{N_{\max}-1}^{(q)} - E_{N_{\max}}^{(q)}$  decrease rapidly on a logarithmic scale. In fact, the decrease is steeper than linear on that scale, suggesting that the convergence might be faster than exponential. The solid lines are quadratic fits to  $\log(\Delta E_{N_{\max}}^{(q)})$ , used to extrapolate to a value of  $E^{(q)} \equiv E_{\infty}^{(q)}$ . We observe the decrease rate of  $\Delta E_{N_{\max}}^{(q)}$  to be monotonically increasing with  $N_{\max}$ , so a conservative lower bound in  $E^{(q)}$  is obtained using a fixed-rate extrapolation above  $N_{\max} = 7$  with an average rate determined by the points  $N_{\max} = 5, 6, 7$ . An upper bound for  $E^{(q)}$  is given by  $E_7^{(q)}$ .

Fig. 2(a) shows the converged or extrapolated energies  $E^{(q)}$  versus  $q$ . These energies are monotonically increasing function of  $q$ . For the new interaction (solid circles), we observe a fast convergence to the known exact value (dotted line). Fig. 2(b) shows the absolute value of the deviation  $\delta E^{(q)} \equiv E^{(q)} - E^{(\infty)}$  from the exact result in a logarithmic scale. The concavity of the curve for the renormalized contact interaction (open circles) indicates the convergence in  $q$  is slower than exponential. We find this convergence to be consistent with a low negative power law  $\sim q^{-\alpha}$  with  $\alpha$  in the range  $\sim 0.5 - 1.5$  (for the excited  $A = 2$  system it can be shown analytically

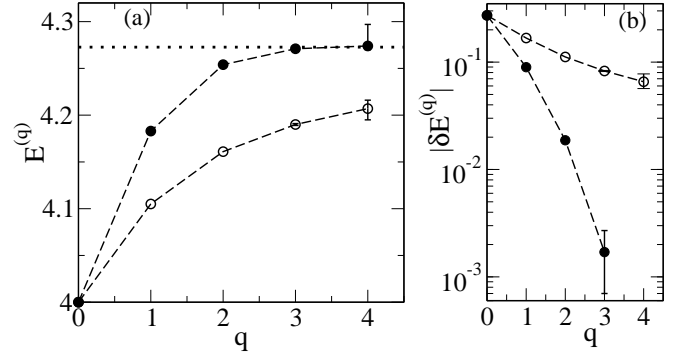


FIG. 2: Convergence of the  $q$ -regulated energies for the  $A = 3$  ground state. (a)  $E^{(q)}$  versus  $q$  for both interactions (symbols and units as in Fig. 1). The dotted line is the exact ground-state energy. (b) The error  $|\delta E^{(q)}|$  in a logarithmic scale.

that  $\alpha = 1/2$ ). However, for the new interaction (solid circles) the convergence is at least exponential.

This exponential convergence allows for an accurate estimate of  $E^{(\infty)}$ . We calculated successive energy differences  $\Delta E^{(q)} \equiv E^{(q-1)} - E^{(q)}$  and determined an average rate of decrease  $\lambda$  of  $|\Delta E^{(q)}|$  for  $q$  below a given  $q'$ . Assuming a fixed rate  $\lambda$  for  $q > q'$ , the extrapolated energy is  $[\lambda E^{(q')} - E^{(q'-1)}]/(\lambda - 1)$ . We can take this value to be an upper bound for  $E^{(\infty)}$ , since the rate of decrease of  $|\Delta E^{(q)}|$  seems to be a monotonically non-decreasing function of  $q$ . Using  $q' = 3$  and an average decrease rate of 3.28 (determined from  $\Delta E^{(q)}$  at  $q = 1, 2, 3$ ), we find  $E^{(\infty)} = (4.274 \pm 0.004)\hbar\omega$ , an accuracy of 0.1%.

We carried out a similar study for the  $L^\pi = 0^+$  first excited state at  $E^{(\infty)} = 4.6662 \dots \hbar\omega$  [4, 13]. Results are shown in Fig. 3(a). As in the ground-state case, we observe a low negative power law convergence for the renormalized interaction and exponential convergence for our interaction. Using  $E^{(3)}$  and an average decrease rate of 1.83 obtained from  $q = 1, 2, 3$ , we estimate  $E^{(\infty)} = (4.646 \pm 0.025)\hbar\omega$ , an accuracy better than 0.6%.

*A=4 system.* We also studied the  $L = 0$  ground state of the  $A = 4$  system with two particles of each species. The results for  $E^{(q)}$  are shown in Fig. 3(b). Here the exact value  $E^{(\infty)}$  is unknown. An upper bound (using the new interaction) is  $E_7^{(3)} = 5.075 \hbar\omega$ . A lower bound can be obtained as for the  $A = 3$  system. The inset of Fig. 3(b) shows  $\Delta E^{(q)}$  in a logarithmic scale versus  $q$  for the new interaction. Again, the convergence seems to be at least exponential. The straight line is a fit to  $\log(\Delta E^{(q)})$  using  $q = 1, 2, 3$ , and provides an average decrease rate of 2.14. Using the extrapolated  $E^{(3)} = (5.074 \pm 0.001)\hbar\omega$  and this average rate, we estimate  $E^{(\infty)} = (5.051 \pm 0.024)\hbar\omega$ . Our result agrees with fixed-node Monte Carlo estimates of  $(5.1 \pm 0.1)\hbar\omega$  [1] and  $(5.069 \pm 0.009)\hbar\omega$  [2].

*Discussion.* There are a number of methodologies in current use to construct effective interactions for many-particle systems; among them, effective field theory

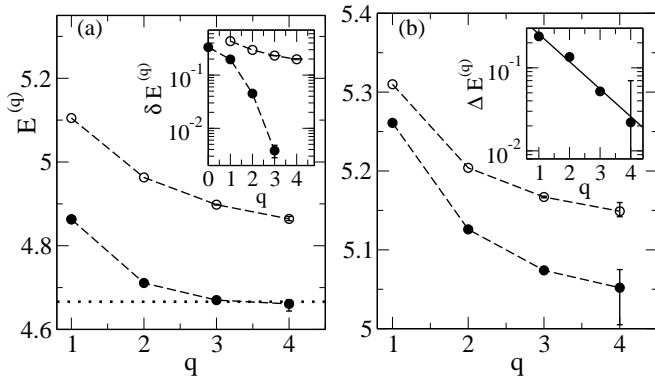


FIG. 3: (a)  $E^{(q)}$  versus  $q$  for the lowest  $L = 0$  excited state of the  $A = 3$  system. The inset shows  $\delta E^{(q)}$  versus  $q$  in a logarithmic scale. Symbols and units as in Fig. 2. (b)  $E^{(q)}$  versus  $q$  for the  $L = 0$  ground state of the  $A = 4$  system. The inset shows  $\Delta E^{(q)}$  versus  $q$  for the new interaction in a logarithmic scale. The solid line is a linear fit to  $q = 1, 2, 3$ .

(EFT) and the unitary-transformation method have a connection to the interactions discussed here. In EFT, the interaction is parameterized by contact terms (leading order) and their derivatives. Our procedure to construct the  $q$ -renormalized contact interaction can thus be considered as leading-order EFT. Its poor convergence suggests that EFT treatments will require derivative terms to accurately model trapped fermion systems.

Our improved interaction has some connection with Suzuki's unitary regularization [14], a method widely used in nuclear physics [15, 16, 17]. In Suzuki's approach, an effective interaction is determined by a unitary transformation of the Hamiltonian that decouples a subspace from its complementary subspace. In practice, the transformation is performed on the two-particle Hamiltonian, giving a transformed Hamiltonian that is block diagonal. This block diagonal structure guarantees that the energy eigenvalues are reproduced in the truncated subspace. Our effective interaction also reproduces the exact two-particle spectrum in a truncated subspace but has the advantage of being simple, i.e., separable.

The unitary transformation of the two-particle Hamiltonian cannot be carried out independently for all possible pairings in the many-body Hamiltonian. When this transformation is applied to the many-particle system, it generates higher-order many-body interactions that are usually simply neglected. For our Hamiltonian, additional correction terms would be required if we were to relate it to a unitary-transformed Hamiltonian. Rather than attempting to compute these correction terms, we have studied the convergence in the large  $q$ -limit, where our effective interaction coincides with the contact interaction. By studying the convergence, one can assess the usefulness of many of the specific details of the different methodologies. For example, there are other choices of the many-particle space truncation that might be more

efficient. Non-unitary transformations might give faster convergence. The no-core-shell-model methodology [18] is an example where a particular choice was made.

Our method can be applied for interaction strengths away from unitarity, at the slight cost of inverting numerically a  $(q + 1)$ -dimensional matrix. It may also be interesting to apply the method to uniform systems, using the separability of the interaction in a plane-wave basis. One caveat is that we have only examined three- and four-particle systems. It will be important to confirm the exponential convergence when our interaction is used to calculate the spectra of systems with more particles.

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- [1] S.Y. Chang and G.F. Bertsch, arXiv: physics/0703190.
  - [2] J. von Stecher, C.H. Greene, and D. Blume, arXiv:0705.0671.
  - [3] A. Bulgac, arXiv:cond-mat/0703526.
  - [4] F. Werner and Y. Castin, Phys. Rev. Lett. **97**, 150401 (2006).
  - [5] The spectrum is most easily derived by noting that the boundary condition  $(u'/u)|_{r=0} = 0$ , imposed by the unitary interaction on the radial wave function  $u(r)$ , effectively maps the 3-D  $s$ -wave problem onto the even solutions of the 1-D harmonic oscillator.
  - [6] T. Busch, et al., Foundations of Physics, **28**, 549 (1998); S. Jonsell, Few-Body Systems **31**, 255 (2002).
  - [7] While writing up this manuscript, we learned of I. Stetcu, B.R. Barrett, U. van Kolck, and J.P. Vary, arXiv:0705.4335, which uses a similar truncation.
  - [8] The sum in (7) can be performed analytically to give  $\chi_q^{-1} = -2\pi^{-2}\Gamma(q + \frac{3}{2})/\Gamma(q + 1) \approx -2\sqrt{(q + 3/4)}/\pi^2$ .
  - [9] A. Bulgac, J. E. Drut, and P. Magierski, Phys. Rev. Lett. **96**, 090404 (2006).
  - [10] Fortunately the solutions  $f_n^2$  are all positive; otherwise the construction would fail.
  - [11] I. Talmi, Helv. Phys. Acta **25**, 185 (1952); M. Moshinsky, Nucl. Phys. **13**, 104 (1959).
  - [12] B.A. Brown, A. Etchegoyen, and W.D.M. Rae, MSU-NSCL Report **524** (1988).
  - [13] S. Tan, arXiv:cond-mat/0412764; D.S. Petrov, C. Salomon, and G.V. Shlyapnikov, Phys. Rev. Lett. **93**, 090404 (2004).
  - [14] K. Suzuki, Prog. Theor. Phys. **68**, 246 (1982).
  - [15] N. Barnea, W. Leidemann, and G. Orlandini, Phys. Rev. C **61**, 054001 (2000).
  - [16] S. Fujii, R. Okamoto, and K. Suzuki, Phys. Rev. C **69**, 034328 (2004).
  - [17] C. Barbieri, Phys. Lett. B **643**, 268 (2006).
  - [18] P. Navrátil, J. Vary, and B. Barrett, Phys. Rev. C **62**, 054311 (2000).